Value of the CAPE-OPEN standard for ATOFINA

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Outline

Introduction

- ATOFINA/TotalFinaElf commitment to CAPE-OPEN
- CAPE-OPEN standard status
- Vor directions, policy, requirements
- Achievements
- Conclusion

TotalFinaElf at a glance

- World's fifth-largest oil and gas company
 - Production: 2,197,000 barrels of oil equivalent per day
 - Proven reserves at end-2001: 10,978 million barrels of oil equivalent
- Europe's front-ranked refiner and marketer
 - 27 refineries
 - 16,900 service stations
- France highest market capitalization
- ATOFINA: world's sixth largest chemicals manufacturer

Key Positions- Chemicals

ATOFINA is the world's sixth-ranked chemical manufacturer

- Chemical sales outside the Group: €19.6 billion (of which 65% in Europe)
 - Petrochemicals and commodity polymers: €7 billion
 - Intermediates and performance polymers: €4.7 billion
 - Specialty chemicals: €7.8 billion
- Capital expenditure: €1.6 billion
- 71,312 employees, including 5,500 researchers

Sales by Business

2001 Sales by Business

Petrochemicals and Commodity Polymers

- Aromatics/Butadiene
- Steamcracking/Olefins
- Polyethylene
- Polypropylene
- Styrene
- Vinyl products
- Vinyl compounds

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- Pipes and steel sections
- Fertilizers



Intermediates and performance polymers

- Chlorine, vinyl and solvents
- Fluorinated & oxygenated
- Acrylics-PMMA
- Thiochemicals and fine chemicals
- Organic peroxides
- Industrial specialties
- Additives
- Formaldehyde resins
- Agrochemicals
- Engineering polymers
- Complex films

Worldwide Chemicals Operations

30 Asian plants

200 European plants

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100 plants in the Americas

ATOFINA Process Simulation Team

- Missions within ATOFINA
 - Specifies, deploys and supports process modeling software tools within ATOFINA business units
- Actions within TotalFinaElf
 - Leads Modeling & Simulation working party in corporate Process Engineering network of TotalFinaElf
 - Provides consultancy on software architecture to the upstream business
 - Represents TotalFinaElf in CAPE-OPEN projects and related organizations since the start

An array of simulation tools

1		Chemicals (ATOFINA)	Refining & Marketing	Upstream
	Aspen Plus	X		
	HYSYS		X	
	PRO II		X	X

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CAPE-OPEN standard

- CAPE-OPEN is a standardization process for achieving true plug and play of process industry simulation software components
- An industrial answer to:
 - Limited reuse of third-party models and software
 - Limited interoperability between software tools
- An initiative developed through already 7 years of collaborative work between end-users, suppliers and academics

Our commitment: over \$700 K

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0.9 (CAPE-OPEN) 0.93 (GCO 2001) The CAPE-OPEN standard 1.0 (GCO 2002) Future releases **CO** Simulator Executive Services Simulation context **External Interaction** Other **Business Interfaces** Session Services Planning Operations Physical **SMST** & Scheduling & Control Electrolytes Properties Reactions Numeric PEDR Petroleum Hybrid Solvers Polymers Fractions Unit Thermodynamic and Physical Optimisation **PDAE** Hybrid Units Operations Properties MILP, MINLP Solvers **Physical Properties Solvers Unit Operations** Data Banks LAE, NLAE, DAE **Common Interfaces** Collections Persistence Parameters Identification Known Objects Utilities **Error Handling** Types and undefined values 11

We capitalize on:

What exists as the CO standard

- 0.9 0.93 1.0 1.1 versions
- What CO Simulator Executive providers have implemented
 - UNIT and Thermo sockets in Aspen Plus, HYSYS, PRO II, etc...

What the software market is presently developing

- HTRI: heat exchanger software as CO UNIT plugs
- DECHEMA e.V.: data banks as CO PPDB plugs

Policy enforced

Software development:

- CAPE-OPEN standard compliance included in the specs
 - OTC 2002 Deep offshore well metering and permutation testing

Software purchase:

- CAPE-OPEN standard compliance included in the requirements to be fulfilled
- Priority given to suppliers implementing CO standard

Targeted parts of CO standard

Chemicals

- UNIT Operations
- Thermo Packages
- Physical Properties Data Banks
- Refining & Marketing
 - UNIT Operations
- Vpstream
 - UNIT Operations
 - Thermo Packages
 - Solvers

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Requirements on implementations

VIT Operations

Use of design specs with CO Unit Operations

Thermo Packages

Let model parameters be accessible for fitting data

Data Banks

 Implementation of Physical Properties Data Banks part of CO standard in COSEs

Overall achievements

While it has been recently challenged, CAPE-OPEN is still the only standard for CAPE simulation tools

CAPE-OPEN has achieved commercial status

Performance issues are implementation issues

Benefits from CAPE-OPEN standard

- Benefits for suppliers
 - Increased usage of CAPE tools
 - Reduced development costs
- Benefits for users
 - Have it developed once, and it runs everywhere
 - Access to best-in-class solutions
- Benefits for academics
 - Improved dissemination of research results
 - Better adaptation to industrial needs